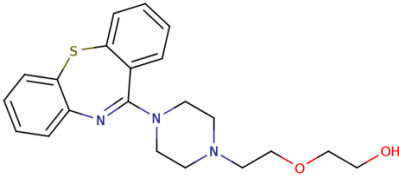
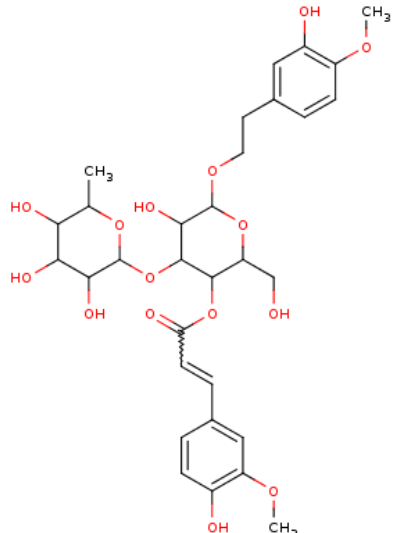
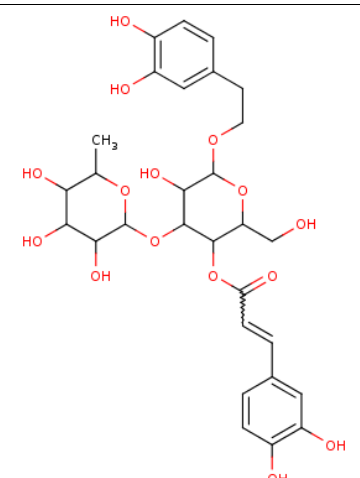
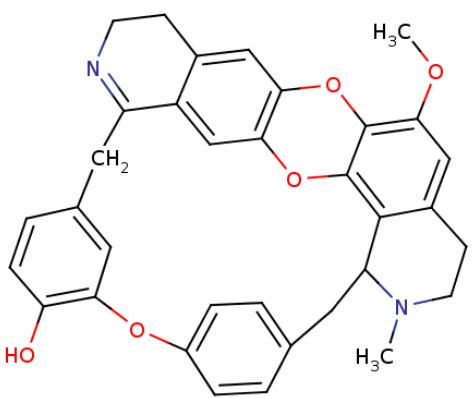


Table S3: Selected natural compounds chemical and structural information.

S.No.	Natural compounds IDs	IUPAC name	SMILES	2D Structures
1.	Drug as a Control Quetiapine	2-[2-(4-benzo[b][1,4]benzothiazepin-6-yl)piperazin-1-yl]ethoxy]ethanol	<chem>C1CN(CCN1CCOCCO)C2=NC3=CC=CC=C3SC4=CC=CC=C42</chem>	 The chemical structure of Quetiapine is shown. It features a benzothiazine core system. A piperazine ring is attached to the benzothiazine at the 4-position. The piperazine ring is further substituted with a 2-(4-hydroxyphenoxy)ethyl group at the 1-position.
2.	STXBP1_CID:5319292 Martynoside	[(2 <i>R</i> ,3 <i>R</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>R</i>)-5-hydroxy-6-[2-(3-hydroxy-4-methoxyphenyl)ethoxy]-2-(hydroxymethyl)-4-[(2 <i>S</i> ,3 <i>R</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>S</i>)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-3-yl] (<i>E</i>)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate	<chem>CC1C(C(C(C(O1)OC2C(C(OC(C2OC(=O)C=CC3=CC(=C(C=C3)O)OC)CO)OCCC4=CC(=C(C=C4)OC)O)O)O)O</chem>	 The chemical structure of Martynoside is shown. It is a complex molecule consisting of a central glycosidic linkage between two sugar units. The left sugar unit is a hexose derivative with multiple hydroxyl groups and a methyl group. The right sugar unit is a hexose derivative with a hydroxyl group and a methyl group. The two sugar units are linked via an ester bond. The structure also includes a phenyl ring with a hydroxyl group and a methyl group.

3.	STXBP1_CID:5281800 Acteoside	[(2 <i>R</i> ,3 <i>R</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>R</i>)-6-[2-(3,4-dihydroxyphenyl)ethoxy]-5-hydroxy-2-(hydroxymethyl)-4-[(2 <i>S</i> ,3 <i>R</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>S</i>)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-3-yl] (<i>E</i>)-3-(3,4-dihydroxyphenyl)prop-2-enoate	<chem>CC1C(C(C(C(O1)OC2C(C(OC(C2OC(=O)C=CC3=CC(=C(C=C3)O)O)CO)OCCC4=CC(=C(C=C4)O)O)O)O)O</chem>	
4.	STXBP1_CID:44559250 Dehydroapateline	(21 <i>S</i>)-27-methoxy-22-methyl-15,29,31-trioxa-7,22-diazaoctacyclo[19.9.3.2 ^{16,19} .1 ^{4,30} .1 ^{10,14} .0 ^{3,8} .0 ^{25,33} .0 ^{28,32}]heptatriaconta-1(30),2,4(34),7,10(37),11,13,16,18,25,27,32,35-tridecaen-13-ol	<chem>CN1CCC2=CC(=C3C4=C2C1CC5=CC=C(C=C5)OC6=C(C=CC(=C6)CC7=NCCCC8=CC(=C(O4)C=C87)O3)O)OC</chem>	

5.	STXBP1_CID:5291488 Luteolin 7-galactoside	2-(3,4-dihydroxyphenyl)-5-hydroxy-7-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	<chem>C1=CC(=C(C=C1C2=CC(=O)C3=C(C=C(C=C3O2)OC4C(C(C(C(O4)CO)O)O)O)O)O</chem>	
6.	STXBP1_CID:11145924 Bacopaside C	[(3 <i>S</i> ,4 <i>R</i> ,5 <i>S</i>)-5-[(2 <i>R</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-4,5-dihydroxy-6-(hydroxymethyl)-2-(2-phenylethoxy)oxan-3-yl]oxy-3,4-dihydroxyoxolan-3-yl]methyl 4-hydroxybenzoate	<chem>C1C(C(C(O1)OC2C(C(C(OC2OCCC3=CC=CC=C3)CO)O)O)O)(COC(=O)C4=CC=C(C=C4)O)O</chem>	
7.	STXBP1_CID:15922618 Bacopaside III	[(2 <i>R</i> ,3 <i>S</i> ,4 <i>S</i> ,5 <i>R</i> ,6 <i>S</i>)-6-[(2 <i>S</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i>)-3,5-dihydroxy-2-[[[(1 <i>S</i> ,2 <i>R</i> ,5 <i>R</i> ,7 <i>S</i> ,10 <i>R</i> ,11 <i>R</i> ,14 <i>R</i> ,15 <i>S</i> ,16 <i>S</i> ,17 <i>R</i> ,20 <i>R</i>)-16-hydroxy-2,6,6,10,16-pentamethyl-17-(2-methylprop-1-enyl)-19,21-dioxahexacyclo[18.2.1.0 ^{1,14} .0 ^{2,11} .0 ^{5,10} .0 ^{15,20}]tricosan-7-yl]oxy]oxan-4-yl]oxy-3,4,5-trihydroxyoxan-2-yl]methyl hydrogen sulfate	<chem>CC(=CC1COC23CC4(CO2)C(C3C1(C)O)CCC5C4(CCC6C5(CCC(C6(C)C)OC7C(C(C(CO7)O)OC8C(C(C(C(O8)COS(=O)(=O)O)O)O)O)C)C)C</chem>	

8.	STXBP1_CID:11091080 Monnieraside I	[(2 <i>R</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-4,5-dihydroxy-6-(hydroxymethyl)-2-[2-(4-hydroxyphenyl)ethoxy]oxan-3-yl] 4-hydroxybenzoate	<chem>C1=CC(=CC=C1CCOC2C(C(C(C(O2)CO)O)OC(=O)C3=CC=C(C=C3)O)O</chem>	
9.	STXBP1_CID:9847922 Plantainoside B	[(2 <i>R</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-2-[2-(3,4-dihydroxyphenyl)ethoxy]-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl] (<i>E</i>)-3-(3,4-dihydroxyphenyl)prop-2-enoate	<chem>C1=CC(=C(C=C1CCOC2C(C(C(C(O2)CO)O)OC(=O)C=CC3=CC(=C(C=C3)O)O)O)O</chem>	
10.	STXBP1_CID:163188454 NA	[(2 <i>R</i> ,3 <i>R</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>R</i>)-4-[(2 <i>S</i> ,3 <i>R</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>R</i>)-3,4-dihydroxy-6-(hydroxymethyl)-5-methyloxan-2-yl]oxy-5-hydroxy-6-[2-(3-hydroxy-4-methoxyphenyl)ethoxy]-2-(hydroxymethyl)oxan-3-yl] (<i>E</i>)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate	<chem>CC1C(OC(C(C1O)O)OC2C(C(OC(C2OC(=O)C=CC3=CC(=C(C=C3)O)OC)CO)OCCC4=CC(=C(C=C4)OC)O)O)CO</chem>	